

A SHORT REVIEW ON CONSTITUTIVE MODELLING OF THE SHAPE MEMORY ALLOYS-1

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ABSTRACT

Shape memory alloys (SMAs) received significant attention by biomedical, aerospace and automotive industries due to their captivating properties called shape memory effect (SME) and Pseudo elasticity. However, the applications of these alloys are mostly found to be biocompatible, and are very sensitive to aerospace and automotive applications. This realization of developing the materials amenable to both aerospace and automotive applications along with biomedical applications needs an assignment of developing suitable constitutive model, to understand the behavior of these materials in different environments. As a result, the present paper emphasizes a short review on various constitutive models, cited in the global scientific community allowing to understand the significance of shape memory alloys, and also suggests essential facts required for developing new models.

KEYWORDS: Shape Memory Effect, Pseudo Elasticity, Constitutive Models, Free Energy & Nitinol

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INTRODUCTION

Recently, SMAs received huge attention by aerospace and automotive industries because of its intriguing properties, say Pseudo elasticity and SME. But, most of these SMAs are constrained to biomedical applications because of their compatibility; hence they cannot be directly integrated with aerospace and automotive industries. These industries require properties like high strength to weight ratio, high thermal resistance and corrosion resistance which requires different processing methodologies unlike those for biomedical industries. Present challenges in processing these alloys received a substantial attention because of unavailability of proper constitutive mechanics to identify the material behavior for different alloying composition. Nonetheless, significant work has been done for various processing methodologies influencing the properties of Nitinol SMA and developed constitutive relations in these aspects. The present section will emphasize few research works performed over the years in deduce the mechanism of these alloys, and also highlights the research gaps identified from the literature review.

REVIEW OF CONSTITUTIVE MODELS

During 1980's, which is the early phases of articulating and modeling of the SME, engineers and scientists found a close analogy with ferroelectric bodies due to the similar hysteretic behavior. As a result, Müller and Wilmanski (1) proposed a macroscopic model to understand the behavior of the hysteresis with ferroelectric bodies. The primary objective of Müller and Wilmanski model is to simulate a body under uniaxial

tensile or compressive loading, by statistical mechanical approach to calculate the free energy and entropy of the system given by equation(1-1). Alongside, they also explained load-deformation and deformation-temperature curves, but the paper couldn't explain the elastic modulus (E) at the origin against the temperature, as shown in Figure 1. However, the paper credits the modelling of lattice structure using statistical ensemble average model, which intended the basis for signifying the phase transitions in Pseudo elastic bodies.

$$\begin{aligned}\varphi_{pot}(D, T) &= -NkT[\ln 2zJ + \beta J \frac{\sqrt{2}D}{NJ} + \ln \frac{1}{J} \int_0^J \left(1 - \frac{\phi(\Delta)}{kT}\right) \cosh \beta \Delta d\Delta], \\ \varphi_{pot}(D, T) &= (E_{0pot} + \sum_{\Delta, \Delta=-\infty}^{\infty} \phi(\Delta) N_{0, \Delta}) - TH_0\end{aligned}\quad (1-1)$$

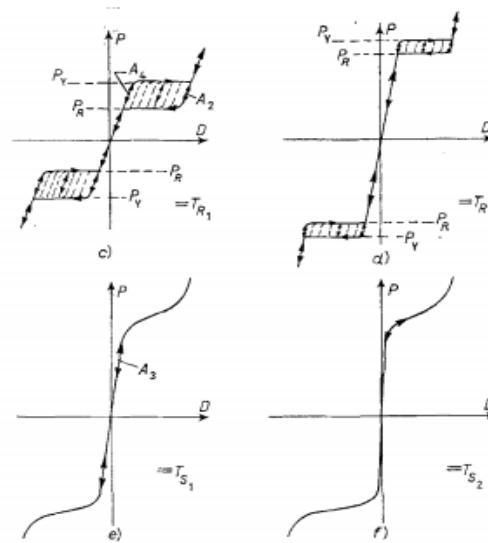


Figure 1: Load Deformation Curve for Intermediate Temperatures (C, D) and High Temperatures (E, F)

Nevertheless, to ascertain the concept of free energy, an enhanced micro model is earmarked already on the basis of stress-strain curves and latent heat of phase transition with shear strain \mathbf{E} by (2), which is well known for Falk's Model. The only drawback Falk's model account for is, constraining the martensite variants during phase transition by Schmid's law (3). The Helmholtz free energy F per volume as a function of shear strain \mathbf{E} and temperature T in Gibbs free energy is specified in

$$G = F - \sum E; \text{ rescaled to } g = f - \sigma e$$

$$\text{Where } F(E, T) = \alpha E^6 - \beta E^4 + (\delta T - \gamma) E^2 + F_0(T)$$

$$f = \frac{\alpha^2}{\beta^3} F e = \left(\frac{\alpha}{\beta}\right)^{\frac{1}{2}} E t = \frac{\alpha \delta}{\beta^2} T - \frac{\gamma \alpha}{\beta^2} - \frac{1}{4} \quad (1-2)$$

Where α , β and γ need to be determined experimentally, and at the same time, these values are completely dependent on the composition strictly.

Jurgen Sprekels (4) proposed a similar model (2) for a one dimensional constitutive model using non-convex potentials of (5), which particularly connects with B2-M phase transitions. The free energy F is defined in Ginzburg-Landau form as given in equation (1-3).

$$F(\epsilon, \epsilon_x, \theta) = -C_V \theta \log\left(\frac{\theta}{\theta_2}\right) + C_V \theta + \tilde{C} + k_1(\theta - \theta_1)\epsilon^2 - k_2\epsilon^4 + k_3\epsilon^6 + \frac{\gamma}{2}\epsilon^2 \quad (1-3)$$

Where k_1, k_2, k_3, γ are constants to be derived, experimentally. From the drawbacks of Falk's model, a rheological model of stress-temperature is constructed by (6) as shown in Figure 2, which accounts the equivalent direction and magnitude of critical lower shear stress from the energy equations.

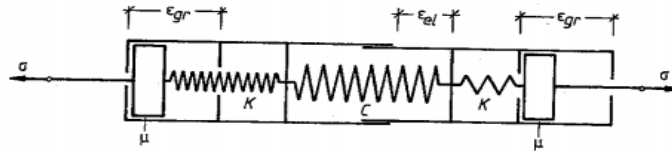


Figure 2: Rheological Model

Where, material is entirely idealized by elastic springs (Hookean elasticity) and dry friction element (plastic/St.-Venant) defining temperature dependence stiffness $C(T)$, $K(T)$ and friction coefficients $\mu(T)$ given by relations in equation

$$\sigma_{F_1} = K(T) + \mu(T), \sigma_{F_2} = K(T) - \mu(T)$$

Energy Stored in elastic spring $\frac{1}{2} C \epsilon_{el}^2$ and in

Pre-strained springs $K \epsilon_{pl}$ (1-4)

The only drawback that paper accounts for is the absence of strain hardening resulting in the following cases

$$\left. \begin{array}{l} \text{For low temperature } K = 0 \\ \text{For high temperature } \mu = 0 \end{array} \right\} \begin{array}{l} \text{in the absence of} \\ \text{strain hardening} \end{array}$$

It is intriguing to understand intuitive nature of SMA to detect their yield point by simple stretch test. Theories like Gibbs free energy, Falk's model and other models couldn't explain the phenomena of yielding. General assumption of yield point from Gibbs energy concept suggests that discontinuities of deformation or stretch are observed, but the case of SMA doesn't obey this concept because of its Pseudo elasticity. In this context, (7) proposed a model to predict the yield point by using Maxwell line with stress as a function of temperature given by equation

$$\tau^* = \tilde{\tau}^*(\theta_e) \quad (1-5)$$

Later the work from (7), Falk (8) realized that domain wall motion is responsible for SME followed by the phase transformation, and hence investigated the domain wall motion under the influence of external shear forces. In his subsequent paper (9), he realized the importance of domain walls (where strain jumps) by assuming them as shock waves because of their small thickness. By introducing the shock waves into constitutive equation(1-2, shear stress is determined and is given by the equation (1-6

$$\sigma(E, T) = \frac{\partial F(E, T)}{\partial E} = 6E^5 - 4E^3 + 2\gamma(T)E, \sigma(E, S) = \frac{\partial F(E, S)}{\partial E} = 6E^5 - 4E^3 + 2\gamma(S)E \quad (1-6)$$

It is important to know the magnitude of the phase transition, through which continuous-cooling-transformation (CCT) and time-temperature-transformation (TTT) diagram can be derived, a work in this pretext is already available by

constructing a constitutive model using continuum mechanics which can be reviewed from (10). This is the first macroscopic Phenomenological model developed to understand solid-solid phase transition and named as Tanaka model. The general thermo-constitutive equation for any material in a stress-strain state is given by

$$\bar{\sigma} = \frac{\partial \sigma}{\partial \bar{\varepsilon}} \dot{\bar{\varepsilon}} + \frac{\partial \sigma}{\partial T} \dot{T} + \frac{\partial \sigma}{\partial \xi} \dot{\xi} = D \dot{\bar{\varepsilon}} + \Theta \dot{T} + \Omega \dot{\xi}$$

$$\text{Where, } \begin{cases} D = \rho_0 \frac{\partial^2 \Phi}{\partial \bar{\varepsilon}^2} \\ \Theta = \rho_0 \frac{\partial^2 \Phi}{\partial \bar{\varepsilon} \partial T} \\ \Omega = \rho_0 \frac{\partial^2 \Phi}{\partial \bar{\varepsilon} \partial \xi} \end{cases} \quad (1-7)$$

Substituting the internal energy in first law of thermodynamics, will result in equation (1-77, which yield the expression for rate of entropy as

$$\left(\frac{\bar{\sigma}}{\rho_0} - \frac{\partial \Phi}{\partial \bar{\varepsilon}} \right) \dot{\bar{\varepsilon}} - \left(S + \frac{\partial \Phi}{\partial T} \right) \dot{T} - \frac{\partial \Phi}{\partial \xi} \dot{\xi} - \frac{1}{\rho_0 T} f^{-1} q^{sur} \frac{\rho_0}{\rho} \frac{\partial T}{\partial X} \geq 0 \quad (1-8)$$

The generalized form of equation (1-8 is given below and is known as Hoffman's-Sprekel's model (11).

$$\Phi(\varepsilon, \Theta) = \Phi_0(\Theta) + \Phi_1(\Theta)\varepsilon^2 + \Phi_2(\varepsilon) \quad (1-9)$$

Linear 1-D models have been developed so far to understand the SME, but during unloading at B2 state, doesn't give the same path in hysteresis, but still behave like a complimentary shear. It indicates that there is energy dissipation which doesn't allow the system amenable to apply basic second law of thermodynamics to understand SME. Therefore, a new term is added as dissipation state function to this law, and developed a non-equilibrium thermostatic model for stress-strain B2M path as given by

$$F_{BAM} - F = (F_{BAMx} - F_x) \exp \left| \frac{g(T-T_x) - f(L-L_x)}{F_{BAMx} - F_x} \right| \quad (1-10)$$

It is an imperative model developed by (12) which decomposes the strain tensor into elastic strain ϵ_{ij}^e (obey Hooks law for B2 & M) and inelastic strain ϵ_{ij}^u (governed by normality theory of plastic theory) given as

$$\text{Elastic } \epsilon_{ij} = \epsilon_{ij}^e + \epsilon_{ij}^u, \text{ Inelastic } d\epsilon_{ij}^u = d\lambda \frac{\partial f}{\partial s_{ij}} \quad (1-11)$$

Extending the work of Tanaka model (10), Liang (13) expressed equation (1-7 in integral form by assuming D, Θ, Ω as constants resulting in equation (1-12.

$$\bar{\sigma} - \bar{\sigma}_0 = D(\bar{\varepsilon} - \bar{\varepsilon}_0) + \Theta(T - T_0) + \Omega(\xi - \xi_0) \quad (1-12)$$

Unlike Tanka model, Liang considered Martensitic Volume fraction as an expression of cosine and exponential form, which enable the model to understand SME in SMA more clear form. The model is named after his name as Liang's model. The above research is produced over the decade 1980-1990 is basically on the modelling of martensitic transformation temperature, shear stress, shear strain relations followed by slight emphasis on hysteretic behavior. But few models lack traces of experimental evidences, which were produced over the next decade i. e., 1990-2000. To discuss works on different parameters influencing the constitutive model, (14) established a critical experimental work to

understand factors effecting SME such as ageing of martensite on shape-strain degradation by subjecting to number of thermal cyclic loadings, but the work didn't emphasize the mathematical modelling, and hence didn't receive much attention.

Otsuka (15) envisaged about the limits of stress and strain where complete strain/shape recovery can be attained. He explained this in terms of stress induced transformations (crystallography of martensitic transition) and its thermodynamics. The shape strain than can be written as $P_1 = RP_2B$, when resolved into parallel and normal to invariant plane such that,

$$m_1 d_1 = m_1^p d_1^p + m_1^n p_1 \quad (1-13)$$

Where, $m_1^p d_1^p$ and $m_1^n p_1$ represent shear and dilatational components respectively and the meaning of the equation (1-13). Since it is a plane strain problem, by using Mohr's circle, the external work done can be expressed in terms of plane stress and habit plane orientation as

$$\Delta G^s = \frac{1}{2} |\sigma_a| [m_1^p \sin 2\varphi \pm m_1^n (1 + \cos 2\varphi)] \quad (1-14)$$

The thermodynamic stress-induced transformation than can be given as equation (1-15 called as Clausius-Clapeyron relation.

$$\frac{\partial \sigma}{\partial T} = -\frac{\Delta S^{P-M}}{\varepsilon^{P-M}} = -\frac{\Delta H^{*P-M}}{T_0(\sigma)\varepsilon^{P-M}} = -\frac{\Delta Q(\sigma)}{T_0(\sigma)\varepsilon^{P-M}} \quad (1-15)$$

Transformation strain is calculated based on the orientation dependence given as

$$\varepsilon = [(m_1^p \sin \chi)^2 + 2m_1^p \sin \chi \cos \lambda + 1]^{\frac{1}{2}} - 1 + m_1^n \sin^2 \chi \quad (1-16)$$

Waymen (12) developed multi-dimensional constitutive model using plastic flow theory whereas Liang (13) developed one dimensional constitutive model; using these two models a multi-dimensional constitutive model based on martensite fraction is developed and tested for nitinol SMA by (16). Using equation (1-7, the constitutive equation can be described by and validated with a SMA specimen subjected to torsion. A more generalized one dimensional constitutive model is developed by Spies (17) with inclusion of thermodynamic potential into Falk's model (18) via variables, such as time-dependent distributed and boundary inputs, viscosity effects, fading thermal memory, local curvature effects and internal variables. This setup allowed the present model to solve all the parameters of Falk's model. The well-posedness of the equation (1-3 is given in the dissertation of (17). The physical essence to the well posedness solution is gives by establishing a continuum model developed by Tanaka (10) and Liang (13) to Spies model (17). Inclusion of martensite internal variable function in equation (1-7, Brinson (19) proposed a new constitutive relation as follows

$$\{d\bar{\varepsilon}\} = \{d\bar{\varepsilon}^e\} + \{d\bar{\varepsilon}^t\} + \{d\bar{\varepsilon}^p\} + \{d\bar{\varepsilon}_T\} \quad (1-17)$$

$$\sigma - \sigma_0 = D(\varepsilon - \varepsilon_0) + \Theta(T - T_0) + \Omega_s(\xi_s - \xi_{s0}) + \Omega_T(\xi_T - \xi_{T0}) \quad (1-18)$$

A model developed by (20) which is inevitably more complicated form, which introduces phase change hardening that can examine partial transformation and transformation hysteresis. The journal follows the constitutive rate equation for elastic response in elastic state and phase transformation followed by the transformation laws. The martensite volume fractions expressed in Liang model (13) defined by equation

(1-7 is derived here as

$$\text{For B2-M, } \xi = \xi_M + \frac{M_S^g - T}{M_S - M_f}, \text{ For M-B2, } \xi = \frac{A_S^g - T}{A_S - A_f} \quad (1-19)$$

In conjunction to the previous works by Liang (13), Rogers (16) and Tanaka (10), (21) presumed D, Θ, Ω to be constant from the equation (1-12 and revised energy equation is given by

$$G(T, \sigma, \xi)_{(T, \sigma) \in \mathcal{L}_1} = \tilde{G}(\sigma) + \hat{G}(T, \xi) \quad (1-20)$$

Later, a constitutive model was developed (22) on the basis of the principle of maximum transformation dissipation which is defined as

$$D^t(\zeta \dot{\mathbf{Y}}) = \max_{\mathbf{C}_a \in \mathcal{C}_{all}} D^t(\mathbf{C}_a; \dot{\mathbf{Y}}), \quad (1-21)$$

Subsequently, the importance of elastic constants, a micro plane model is developed by (23) to configure a constitutive relation between the macroscopic and microscopic scale for the phenomenological models, which yields to

$$\sigma_{ij} = \frac{3}{2\pi} \int_{\Omega} \sigma_N n_i n_j d\Omega + \frac{3}{2\pi} \int_{\Omega} \frac{\sigma_{Tr}}{2} (n_i \delta_{rj} + n_j \delta_{ri}) d\Omega \quad (1-22)$$

$$\varepsilon_{ij} = \frac{3}{2\pi} \int_{\Omega} \varepsilon_N n_i n_j d\Omega + \frac{3}{2\pi} \int_{\Omega} \frac{\varepsilon_{Tr}}{2} (n_i \delta_{rj} + n_j \delta_{ri}) d\Omega \quad (1-23)$$

In compliance to the work by (23) a continuum model is proposed in (24) to model energy storage during martensitic phase transition, in terms of introducing internal variables such as martensitic volume fraction into evolution equations given by

$$\psi_e = \hat{\psi}_e(\theta, E_e, z), \psi_s = \hat{\psi}_s(\theta, \mathbf{Y}_{ei}) \quad (1-24)$$

From the above models, most of the work is based on uniaxial loading which do not have framework that can include orientation mechanism. Since it is difficult to predict the behavior of microscopic behavior based on macroscopic model, intact provision to study this phenomenon of microscopic level is by subjecting the specimen one dimensional, multiaxial proportional and non-proportional loading. An imperious work is established by (25), the specific free energy and dissipation equations for one dimensional, multiaxial proportional and non-proportional model are given by

$$\text{Uniaxial: } \rho\psi = \rho\psi^e(\varepsilon, \varepsilon^{tr}) + \rho\psi^T(T) + \rho\psi^{tr}(\varepsilon^{tr}, T, H)$$

$$\text{Multiaxial: } \rho\psi(\underline{\varepsilon}, T, \underline{\varepsilon}^{tr}, H) = \frac{1}{2}(\underline{\varepsilon} - \underline{\varepsilon}^{tr}) : \underline{\underline{L}} : (\underline{\varepsilon} - \underline{\varepsilon}^{tr}) + \rho C \left[(T - T_0) - T \ln \left(\frac{T}{T_0} \right) \right] + \gamma [\mu z (T - T^*) + H] \quad (1-25)$$

A plastic yield constitutive model is developed by (26) based on plastic yielding, which can estimate the simultaneously recoverable transformation strains and irrecoverable plastic strains. The Gibbs energy for the overall SMA material is given by

$$G(\sigma, T, \varepsilon^t, \xi, g^t, \varepsilon^p, g_A^p, g_M^p, \boldsymbol{\beta}) = (1 - \xi)G^A(\sigma, T, \varepsilon^p, g_A^p, \boldsymbol{\beta}) + \xi G^M(\sigma, T, \varepsilon^p, g_M^p, \boldsymbol{\beta}) + G^{mix}(\sigma, \varepsilon^t, g^t) \quad (1-26)$$

An understanding from the literature can be observed that constraining of parameters is required to unify the thermo-elastic-constitutive equations by coupling at micro and macro-mechanics. After careful validations of the above models quantitatively by (27), (28), (29) and (30) etc., it is realized that different applications and characterization techniques yield different anomalies to the above models. Thus, new constitutive models have been adopted based on the

crystallography planes and their orientations. An outlook provided by (31) which decomposes the system into elastic part which represents stretching and rotation of overall structures and inelastic part, which is governed by generation, growth and annihilation of B2-M fine structure. In such case, the free energy is given by

$$\psi(E^e, \vartheta, \xi) = \frac{1}{2} E^e \cdot C(\xi)[E^e] - (\vartheta - \vartheta_0) A(\xi) C(\xi)[E^e] + \frac{\lambda_t}{\vartheta_t} (\vartheta - \vartheta_T) \xi + \frac{1}{2} \sum_{\alpha, k=1}^N g^{\alpha k} \xi^\alpha \xi^k - c(\vartheta - \vartheta_0) - c \vartheta \ln\left(\frac{\vartheta}{\vartheta_0}\right) \quad (1-27)$$

The paper also concluded the effect of strain rate influencing strain-hardening that it is due effect of thermal effects associated with phase transformations. A qualitative and quantitative correlation is made to understand the above concept. Extending the concept of (31), a constitutive equation for reorientation and detwinning phenomena is developed in (32) by mapping reorientation as movement of interfaces between *habit plane variants* (hvp's) and detwinning as movement of interfaces between *lattice correspondent variants* (lcv's). Neglecting the M-M interaction in the equation (1-27, the driving force on detwinning system and the driving force on hvp reorientation is given by

$$\tau^i \equiv (C^e T^*) \cdot S_0^i, \sigma^{ij} \equiv (C^e T^*) \cdot Z_0^{ij} \quad (1-28)$$

An insight to consider the thermal elastic strain and inelastic strain due to accommodation of twins between martensite variants addition to (12) has been modelled by (33) and total macroscopic strain is given.

$$\begin{aligned} \varepsilon &= \varepsilon^e + \varepsilon^{th} + \varepsilon^t + \varepsilon^{twin} \\ \varepsilon^e &= \mathbf{S} : \boldsymbol{\sigma} \\ \varepsilon^{th} &= \boldsymbol{\alpha}(T - T_{ref}) \\ \varepsilon^t &= f \bar{\boldsymbol{\varepsilon}}^T \\ \boldsymbol{\varepsilon}^{twin} &= f^{FA} \bar{\boldsymbol{\varepsilon}}_{ij}^{twin} \end{aligned} \quad (1-29)$$

CONCLUSIONS

From the above review, it can be presumed that shape memory effect (SME) is modelled microscopically, in a more precise way than the macroscopic hysteresis. The understanding of these alloys in the present paper restricts only to loading parameters to understand the hysteresis, but a more insight of exhibiting SME will be emphasized in the next paper by involving processing parameters.

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